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(21) International Application Number: PCT/SE93/00967 (22) International Filing Date: 12 November 1993 (12.11.93) (30) Priority data: 9203478-4 19 November 1992 (19.11.92) SE (71) Applicant (for all designated States except US): BEROL NOBEL AB [SE/SE]; S-444 85 Stenungsund (SE). (72) Inventors; and (75) Inventors/Applicants (for US only) : DAHLGREN, Lennart [SE/SE]; Mjölmarvägen 4, S-444 95 Ödsmåå (SE). BERGSTRÖM, Karin [SE/SE]; PL 3842, S-442 95 Kungälv (SE).		(74) Agent: ANDERSSON, Rolf; Berol Nobel AB, S-444 85 Stenungsund (SE). (81) Designated States: CA, FI, JP, NO, US, European patent (AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE). Published <i>With international search report.</i> BEST AVAILABLE COPY
(54) Title: USE OF ALKOXYLATE OF 2-PROPYL HEPTANOL (57) Abstract The invention relates to the use of an alkoxylate having the general formula (I): $C_5H_{11}CH(C_3H_7)CH_2O(A)_nH$, wherein A is an alkyleneoxy group having 2-4 carbon atoms and n is 2-16, preferably 3-12, in detergent compositions for degreasing hard surfaces.		

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USE OF ALKOXYLATE OF 2-PROPYL HEPTANOL

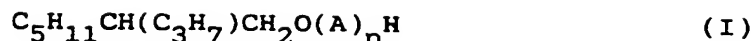
The present invention relates to the use of an alkoxyate of 2-propyl heptanol in compositions for
5 cleaning hard surfaces. The alkoxyate shows low foam-
ing compared with similar compounds having a hydrophobic
group of the same size. The alkoxyate may advantageously
be used as a surface-active component in detergent compo-
sitions.

10 It has long been known to alkoxyate alcohols for
obtaining non-ionic surface-active compounds. These com-
pounds have been used e.g. in detergent compositions
because of their wetting and dispersing properties. In
a number of applications, alkoxyates of C₈₋₁₁ alcohols
15 have however been found to be too high-foaming and/or not
to have the desired detergent power. For example, ethoxy-
lates based on branched C₈ alcohols often exhibit accept-
able foaming but too low a detergent power, whereas
ethoxyates based on straight or branched alcohols having
20 a larger hydrocarbon chain often show an acceptable sur-
face activity but too high foaming. Thus, there is a need
for new alkylene oxide adducts with an improved ratio of
foaming to detergent power.

It has now been found that an alkoxyate based on
25 2-propyl heptanol is suitable for use as a detergent in
compositions for cleaning hard surfaces, since it has good
detergent and wetting properties as well as low foaming as
compared with other alcohols having substantially the same
chain length. In formulations, the alkoxyate also has a
30 desirable thickening effect. In addition, it has been
found that the alkoxyate is easily degradable and has a
surprisingly low biotoxicity. In tests, no skin-irritant
effect has been noted.

The alkoxyate for use according to the invention can
35 be illustrated by the formula

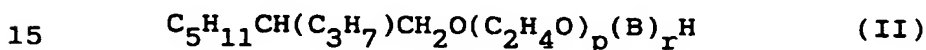
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wherein A is an alkyleneoxy group having 2-4 carbon atoms and n is 2-16, preferably 3-12. Preferably, 50-100% of all alkyleneoxy groups are ethyleneoxy groups. In those cases where different alkyleneoxy groups are present in the same compound, they may be added randomly or in block.

Generally, the alkoxylate is an ethoxylate having 3-7, preferably 4-6 ethyleneoxy groups.

In an advantageous mode of execution, ethylene oxide can be added in a first step and thereafter alkylene oxide having 3-4 carbon atoms. These compounds can be illustrated by the formula



wherein B is an alkyleneoxy group having 3-4 carbon atoms, p is 1-10 and r is 1-6. Preferably, p is 2-8 and r is 1-4. These compounds have lower foaming than the corresponding compounds without any alkyleneoxy groups having 3-4 carbon atoms.

The alkoxylates for use according to the invention described above can be prepared by adding in a conventional manner in the presence of a conventional alkali catalyst, such as potassium hydroxide or sodium hydroxide, the above-mentioned amounts of alkylene oxide to 2-propyl heptanol, which is a so-called Guebert alcohol. According to a preferred mode of execution, the addition of ethylene oxide is performed using a conventional catalyst which gives a narrower distribution of added ethylene oxide than any alkali catalyst, such as NaOH or KOH. Thus prepared alkoxylates according to the invention have very low foaming. Examples of conventional catalysts giving a narrow distribution of added alkylene oxide are $\text{Ca}(\text{OH})_2$, $\text{Ba}(\text{OH})_2$, $\text{Sr}(\text{OH})_2$ and hydrotalcite. The reaction is preferably conducted in the absence of free water to reduce the amount of by-products and usually at a temperature of 70-180°C.

The alkoxyate, especially ethoxyate and alkoxyate of formula II, is suitably included in compositions for cleaning hard surfaces, e.g. for degreasing or dishwashing. Especially good results have been obtained when

5 degreasing lacquered or unlacquered metal surfaces. In addition to the alkoxyate, the compositions may also contain other detergents, such as anionic surface-active compounds. Examples hereof are alkyl sulphate, alkyl ether sulphate, alkyl benzene sulphonate, α -olefin sulphonate

10 and alkyl glyceryl sulphonate. Also, the compositions may contain solutising additives, complexing agents and/or pH-adjusting agents, enzymes, other surface-active components, bactericides and perfumes. The compositions are usually aqueous and in the form of emulsions, microemul-

15 sions or solutions.

The invention will be further illustrated by the following Examples.

Example 1

20 Alkoxyates according to the invention are prepared by alkoxyating 2-propyl ethanol with the amounts of alkylene oxide appearing from the Table below in the presence of potassium hydroxide or $\text{Ca}(\text{OH})_2$ as catalyst. The resulting products were analysed and structurally determined by

25 gas chromatography and mass spectrometry. The turbidity points were measured in water or monobutylether diethylene glycol. The following results were obtained.

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Table 1

Compound	Alcohol	Mole of alkylene oxide/mole of alcohol	Catalyst	Turbidity point	
				Water	BDG
1	2-propyl heptanol	3.0 EO	KOH	-	40
2	2-propyl heptanol	5.5 EO	KOH	-	62
3	2-propyl heptanol	8.4 EO	KOH	60	73
4	2-propyl heptanol	3.0 EO	Ca(OH) ₂	-	29
5	2-propyl heptanol	5.0 EO	Ca(OH) ₂	-	52
6	2-propyl heptanol	7.0 EO	Ca(OH) ₂	-	61
A	2-ethyl hexanol	2 EO	KOH	-	28
B	2-ethyl hexanol	5 EO	KOH	42	-
C	C ₉₋₁₁ alcohol ²⁾	4 EO	KOH	-	62
D	C ₉₋₁₁ alcohol ²⁾	6 EO	KOH	56	-
E	C ₉₋₁₁ alcohol ²⁾	8 EO	KOH	78	-
F	C ₁₁ alcohol ³⁾	3 EO	KOH	-	51
G	C ₁₁ alcohol ³⁾	5 EO	KOH	27	-
H	C ₉₋₁₁ alcohol ²⁾	4 EO	Ca(OH) ₂	-	57

EO = ethylene oxide; PO = propylene oxide,

BDG = monobutylether diethylene glycol

1) PO added first 2) Dobanol 91 from Shell

3) Dobanol 1 from Shell

Example 2

The foaming properties of the alkoxyates reported in the following Table were measured according to Ross-Miles ASTM D 1173-53. The following results were obtained.

Table 2

Compound	Foam height, cm	
	0 min	5 min
2	18	7
4	0	0
5	5	0
6	10	5
A	40	10
B	50	0
C	80	20
D	95	30
E	45	15
H	20	5

From these results it appears that the compounds according to the invention have lower foaming than the most closely related reference products. Thus, compound 2 has lower foaming than compounds A, B, C, D and E, while compounds 4, 5 and 6 have lower foaming than all the reference compounds.

Example 3

On a vertically disposed, lacquered iron plate, smeared with mineral oils, soot, salts and clay was applied 20 ml of a detergent composition made up of the following components.

Parts by weight	Component
34	Compound 6 or H
67	NTA
27	Ethoxylated quaternary fatty amine
20,000	Water

The effect achieved was evaluated both with respect to the area of the cleaned surface (i.e. wettability) and with respect to the cleanness of the cleaned surface. Cleanness was evaluated according to an ascending scale of 1-10, where 1 indicates that no improvement of the cleanliness could be observed and 10 indicates a completely clean surface. The following results were obtained.

Table 3

Compound	Cleaned surface, cm	Cleanness
6	95	9
H	54	8

From these results it appears that the formulation containing the compound according to the invention yielded both improved cleanness and a larger cleaned area.

Example 4

The microtoxicity, which is a measure of the aquatic toxicity, was determined for the compounds below as the water concentration of the compounds at which the ability of luminescent bacteria to emit light for 5 min is reduced by 50%. The following results were obtained.

Table 4

Compound	Concentrate, ppm
2	42
5	31
C	2
D	3
F	1
G	2

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From these results it appears that the compounds according to the invention have essentially lower micro-toxicity than the reference compounds.

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C L A I M S

1. The use of an alkoxylate having the general formula
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$$C_5H_{11}CH(C_3H_7)CH_2O(A)_nH \quad (I)$$
 wherein A is an alkyleneoxy group having 2-4 carbon atoms and n is 2-16, preferably 3-12, in a detergent composition for hard surfaces.
- 10 2. Use as claimed in claim 1, c h a r a c t e r i s - e d in that 50-100% of all the alkyleneoxy groups are ethyleneoxy groups.
- 15 3. Use as claimed in claim 1, c h a r a c t e r i s - e d in that A is ethyleneoxy groups and n is 3-7.
4. Use as claimed in claim 1 or 2, c h a r a c t e r - i s e d by having the formula
 20
$$C_5H_{11}CH(C_3H_7)CH_2O(C_2H_4O)_p(B)_rH \quad (II)$$
 wherein B is an alkyleneoxy group having 3-4 carbon atoms, p is 1-10 and r is 1-6, p preferably being 2-8 and r preferably being 1-4.
- 25 5. Use as claimed in any one of claims 1-4, c h a r - a c t e r i s e d in that the detergent composition is a composition for degreasing unlacquered or lacquered metal surfaces.
- 30 6. An alkoxylate, c h a r a c t e r i s e d by having the formula

$$C_5H_{11}CH(C_3H_7)CH_2O(C_2H_4O)_p(B)_rH \quad (II)$$
 wherein B is an alkyleneoxy group having 3-4 carbon atoms,
 35 p is 1-10 and r is 1-6, p preferably being 2-8 and r preferably being 1-4.

INTERNATIONAL SEARCH REPORT

International application No.

PCT/SE 93/00967

A. CLASSIFICATION OF SUBJECT MATTER

IPC5: C07C 43/11, C11D 1/72

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC5: C07C, C11D

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

SE,DK,FI,NO classes as above

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

CA

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	US, A, 3862243 (THOMAS J. BELLOS), 21 January 1975 (21.01.75) --	1-6
A	US, A, 3340309 (EUGENE A. WEIPERT), 5 Sept 1967 (05.09.67) --	1-6
A	US, A, 2508036 (MILTON KOSMIN), 19 November 1947 (19.11.47) --	1-6
A	US, A, 3567784 (WILLIAM T. TSATSOS ET AL.), 2 March 1971 (02.03.71) --	1-6

☒ Further documents are listed in the continuation of Box C.☒ See patent family annex.

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C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	EP, A1, 0046582 (CONOCO INC.), 3 March 1982 (03.03.82) -- -----	1-6

INTERNATIONAL SEARCH REPORT
Information on patent family members

28/01/94

International application No.

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Patent document cited in search report	Publication date	Patent family member(s)	Publication date
US-A- 3862243	21/01/75	NONE	
US-A- 3340309	05/09/67	BE-A- 683227 DE-A- 1593043 FR-A- 1484951 GB-A- 1131333 NL-C- 134504 NL-A- 6608854	01/12/66 23/07/70 00/00/00 00/00/00 00/00/00 29/12/66
US-A- 2508036	19/11/47	NONE	
US-A- 3567784	02/03/71	NONE	
EP-A1- 0046582	03/03/82	SE-T3- 0046582 CA-A- 1157052 JP-C- 1555089 JP-A- 57042646 US-A- 4302613	15/11/83 23/04/90 10/03/82 24/11/81